Ethyl 2-ethyl-3-hydroxybutanoate
5465-11-2 | DTXSID90282959

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.59e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.07e-01

Confidence level: 5.89e-01

Nearest Neighbors from the Training Set

Image not found
Butyl 3-hydroxypropanoate
Measured: 5.13e-02
Predicted: 1.05e-01

Image not found
Pentyl 2-hydroxypropanoate
Measured: 6.24e-02
Predicted: 1.34e-01

Image not found
Butyl lactate
Measured: 2.74e-01
Predicted: 2.78e-01

Image not found
Propan-2-yl 2-hydroxy-2-methylpropanoate
Measured: 1.03
Predicted: 5.47e-01